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P32038-/GMM/PMC/MEA

2. Patent application number  
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## 3. Full name, address and postcode of the or of each applicant (underline all surnames)

The Queen's University of Belfast  
University Road  
Belfast  
BT7 1NN  
United Kingdom

Patents ADP number (if you know it)

If the applicant is a corporate body, give the country/state of its incorporation

## 4. Title of the invention

"Charged Particle Manipulation"

## 5. Name of your agent (if you have one)

Murgilroyd &amp; Company

"Address for service" in the United Kingdom to which all correspondence should be sent (including the postcode)

Scotland House  
165-169 Scotland Street  
Glasgow  
G5 8PL

Patents ADP number (if you know it)

1198015

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Country

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Claim(s)

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11.

I/We request the grant of a patent on the basis of this application.

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Murgitroyd &amp; Company

Date

27 August 2002

12. Name and daytime telephone number of person to contact in the United Kingdom

Peter McBride

0141 307 8400

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**Patents Form 1/77**

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1 Charged Particle Manipulation

2  
3 The present invention relates to the manipulation of  
4 charged particles, in particular to methods and  
5 apparatus for manipulating the phase space of at  
6 least one charged particle.

7  
8 Trapping of charged particles has a wide range of  
9 potential applications including frequency  
10 standards, quantum computation, quantum encryption  
11 and material processing/fabrication.

12  
13 However, there is a need for such applications to be  
14 easier to realise.

15  
16 According to a first aspect of the present invention  
17 there is provided a method for manipulating the  
18 phase space of at least one charged particle,  
19 wherein a combination of alternating current and  
20 direct current voltages applied to an electrode  
21 forms a potential which provides a region of phase  
22 space manipulation, and wherein the at least one

1 charged particle is situated to one side of the  
2 electrode surface.

3  
4 According to a second aspect of the present  
5 invention, there is provided apparatus for  
6 manipulating the phase space of at least one charged  
7 particle, comprising at least one electrode arranged  
8 on a surface and connected to a power supply capable  
9 of applying both an alternating current voltage and  
10 a direct current voltage so as to form a potential  
11 which provides a region of phase space manipulation  
12 to one side of the electrode surface.

13  
14 Preferably, the apparatus further comprises pressure  
15 control means to control the pressure of the space  
16 surrounding the electrodes.

17  
18 Preferably, the pressure control means comprises a  
19 sealable chamber and gas pump means capable of  
20 introducing and extracting gases from the chamber.

21  
22 Preferably, the power supply is operable to vary the  
23 alternating current and direct current voltages  
24 applied.

25  
26 Preferably, the power supply is operable to  
27 individually alter the amplitude, waveform, and  
28 frequency of the alternating current voltage, and is  
29 operable to alter the magnitude of the direct  
30 current voltage.

31  
32 Preferably, the potential is an effective potential.

- 1 Preferably, the region of phase space manipulation  
2 comprises a particle trapping region, wherein a  
3 particle is constrained in a specific spatial area.  
4  
5 Preferably, the region of phase space manipulation  
6 comprises a particle guide region, wherein a  
7 particle's motion is restrained by at least one  
8 degree of freedom.  
9  
10 Preferably, a plurality of electrodes are provided.  
11  
12 Preferably, the electrodes are arranged in an array  
13 such that the at least one particle is situated to  
14 one side of the array.  
15  
16 Preferably, the array is substantially planar.  
17  
18 Alternatively, the array is hemispherical.  
19  
20 According to a first embodiment of the present  
21 invention, a single electrode is provided, and is  
22 surrounded by a plane held at a constant potential.  
23  
24 Preferably, the electrode is circular.  
25  
26 Preferably, the plane is earthed.  
27  
28 Preferably, the frequency of alternating current  
29 voltage applied to the circular electrode is of a  
30 frequency having a period that is less than the time  
31 taken for light to pass over the diameter of the  
32 circular electrode.

1 According to a second embodiment of the present  
2 invention, the voltages applied to adjacent first  
3 and second sets of electrodes in a planar array can  
4 be varied such that the at least one particle can be  
5 moved from the particle trapping region provided by  
6 the first set of electrodes to the particle trapping  
7 region provided by the second set of electrodes.

8  
9 Each set of electrodes may consist of one electrode,  
10 or of a plurality of electrodes.

11  
12 Preferably, at least one particle is moved from a  
13 first trapping region provided by a first set of  
14 electrodes to a second trapping region provided by a  
15 second set of electrodes, wherein the voltages  
16 applied to the sets of electrodes is changed from an  
17 initial, to an intermediate and then to a final  
18 configuration, and wherein;

19 in an initial configuration, a first set of  
20 electrodes is biased to a holding voltage to form a  
21 first particle trapping region to trap at least one  
22 particle therein, and an adjacent second set of  
23 electrodes is biased to zero volts;

24 in an intermediate configuration, both sets of  
25 electrodes are biased to the holding voltage to form  
26 a merged particle trapping region that traps the at  
27 least one particle;

28 in a final configuration, the first set of  
29 electrodes is biased to zero volts, and the second  
30 set of electrodes is biased to the holding voltage  
31 to form a second particle trapping region, that  
32 traps the at least one particle.

1 Preferably, the process of moving at least one  
2 particle from a first trapping region provided by a  
3 first set of electrodes to a second trapping region  
4 provided by a second set of electrodes is repeatable  
5 to move the at least one particle along a chosen  
6 path on the planar array.

7  
8 The planar array can be formed using printed circuit  
9 board, lithographic, or focussed ion beam  
10 technology.

11  
12 According to a third embodiment of the present  
13 invention, a series of electrodes are provided, the  
14 voltages applied to which are controllable such that  
15 the at least one particle can be moved from a first  
16 particle trapping region to a second particle  
17 trapping region, wherein the first trapping region  
18 is larger than the second trapping region.

19  
20 Preferably, the voltages applied to the electrodes  
21 are controllable such that the at least one particle  
22 can be moved between a plurality of successively  
23 smaller trapping regions.

24  
25 Preferably, the series of electrodes comprises a  
26 plurality of concentrically arranged circular  
27 electrodes.

28  
29 Preferably, in an initial state, every electrode has  
30 a combination of alternating current and direct  
31 current voltages applied such that at least one  
32 particle is trapped in a first trapping region;



1           the voltage applied to the outer electrode is  
2   changed such that, in an intermediate state, the at  
3   least one particle is trapped in a first  
4   intermediate trapping region provided by the  
5   remaining inner electrodes; and  
6           the voltage applied to the electrode adjacent  
7   to the outer electrode is changed such that in a  
8   final state, the at least one particle is trapped in  
9   a second trapping region provided by the innermost  
10   electrode.

11  
12   Preferably, in the transitions from the initial to  
13   intermediate and the intermediate to final states,  
14   the outer and adjacent electrodes respectively are  
15   set to zero volts.

16  
17   Preferably, a plurality of electrodes each provide a  
18   further intermediate trapping region, such that,  
19   between the initial state and the final state, the  
20   at least one particle passes through a plurality of  
21   intermediate states, being trapped in successively  
22   smaller intermediate trapping regions.

23  
24   Preferably, in an initial state, an outermost  
25   electrode has a first combination of alternating  
26   current and direct current voltages applied, and a  
27   background voltage is applied to the remaining  
28   electrodes such that, in an initial state, at least  
29   one particle is trapped in a first trapping region;  
30           the electrode adjacent to the outer electrode  
31   is set to the first combination of voltages and the  
32   background voltage is applied to the outer electrode

1 such that, in an intermediate state, the at least  
2 one particle is trapped in a first intermediate  
3 trapping region; and

4 the innermost electrode is set to the first  
5 combination of voltages and the background voltage  
6 is applied to the adjacent electrode such that, in a  
7 final state, the at least one particle is trapped in  
8 a second trapping region.

9  
10 Preferably, the background voltage is zero volts.

11  
12 Preferably, a plurality of electrodes is provided  
13 such that, between the initial state and the final  
14 state, the at least one particle passes through a  
15 plurality of intermediate states, being trapped in  
16 successively smaller intermediate trapping regions.

17  
18 Preferably, the innermost electrode is provided with  
19 an aperture; and

20 when the at least one particle is in the final  
21 state, a voltage is applied to the aperture such  
22 that the at least one particle is urged through the  
23 aperture.

24  
25 Preferably, each side of the aperture is  
26 differentially pumped so that a gas passing through  
27 the aperture undergoes a supersonic expansion, so as  
28 to cool the particles that are urged through the  
29 aperture.

30  
31 According to a fourth embodiment of the present  
32 invention, the voltages applied to an electrode are

1 such that one type of charged particle can be  
2 distinguished from another.

3  
4 Preferably, different types of charged particle are  
5 trapped at different distances perpendicularly from  
6 the surface of the electrode.

7  
8 Preferably, the distance is dependent on the charge  
9 and/or mass of the charged particle.

10  
11 Preferably, a first type of charged particle is  
12 trapped at a first perpendicular distance from the  
13 electrode, and a second type of charged particle is  
14 trapped at a second perpendicular distance from the  
15 electrode, wherein the mass of the first charged  
16 particle is greater than the mass of the second  
17 charged particle, and the second perpendicular  
18 distance is greater than the first perpendicular  
19 distance.

20  
21 Preferably, at least one particle trapped at the  
22 second perpendicular distance is subject to the  
23 potential formed by a voltage sequence applied to a  
24 second set of electrodes.

25  
26 Preferably, the voltage sequence applied to the  
27 second set of electrodes is such as to transport  
28 said at least one particle from one trapping region  
29 to another along a predetermined path.

30

1 Preferably, the dimensions of the second set of  
2 electrodes are of a much larger scale than the  
3 dimensions of the trap electrode.

4  
5 Preferably, an aperture is provided on an electrode  
6 such that the type of particle that is closest to  
7 the surface of the electrode can pass through the  
8 aperture.

9  
10 Preferably, each side of the aperture is  
11 differentially pumped so that a gas passing through  
12 the aperture undergoes a supersonic expansion, so as  
13 to cool the particles that are urged through the  
14 aperture.

15  
16 According to a fifth embodiment of the present  
17 invention, the voltages applied to an electrode can  
18 be changed such that a trapped particle moves in a  
19 direction perpendicular to the plane of the  
20 electrode.

21  
22 Preferably, at least one trapped particle can be  
23 lowered to a region where it will interact with at  
24 least one other particle; and  
25 the particles that result from the interaction  
26 can then be raised up again, together with particles  
27 that have not interacted.

28  
29 Preferably, the electrode is formed with an aperture  
30 and the applied voltage can be changed to bring a  
31 particle close to the aperture; and

10

1 a voltage is applied to the aperture such that  
2 the particle is urged through the aperture.

3  
4 Preferably, each side of the aperture is  
5 differentially pumped so that a gas passing through  
6 the aperture undergoes a supersonic expansion, so as  
7 to cool the particles that are urged through the  
8 aperture.

9  
10 According to a sixth embodiment of the present  
11 invention, an array of electrodes is provided, the  
12 voltages applied to which trap a first type of  
13 particle which can interact with a second type of  
14 particle, to form a reactant particle which falls to  
15 the bottom of a trap and is swept away through an  
16 extraction hole.

17  
18 According to a further aspect of the present  
19 invention, there is provided apparatus for carrying  
20 out the method of the sixth embodiment, comprising  
21 an array of electrodes arranged on a surface, at  
22 least one of which is connected to at least one  
23 power supply capable of applying both an alternating  
24 current voltage and a direct current voltage,  
25 wherein a region of phase space manipulation is  
26 provided to one side of the electrode surface.

27  
28 Preferably, the array of electrodes further  
29 comprises at least one aperture for the extraction  
30 of trapped particles.

31  
32 Preferably, each electrode comprises one aperture.

11

1 Preferably, the reactant particle is accelerated  
2 through a potential and detected so that the  
3 position of the original first type of particle can  
4 be detected.

5  
6 The present invention will now be described, by way  
7 of example only, with reference to the accompanying  
8 drawings, in which:

9  
10 Fig. 1 illustrates potential contours suitable for  
11 trapping a charged particle formed by an electrode  
12 in accordance with a first embodiment of the  
13 invention;

14  
15 Fig. 2 illustrates a third embodiment of the  
16 invention;

17  
18 Fig. 3 illustrates potential contours where a  
19 particle will not be trapped;

20  
21 Fig. 4 illustrates a fourth embodiment of the  
22 present invention;

23  
24 Fig. 5 illustrates apparatus used in accordance with  
25 all embodiments of the invention; and

26  
27 Fig. 6 illustrates a sixth embodiment of the  
28 invention.

29  
30 In the adiabatic approximation, a particle of mass  $m$   
31 and charge  $q$  subject to a set of DC and rapidly  
32 varying AC voltages (angular frequency  $\Omega$ ) applied

12

1 to a series of electrodes moves as if subject to an  
 2 effective potential  $V^*$  which is a linear combination  
 3 of an AC term and a DC term, and takes the form

$$4 \quad V^*(R_0) = q^2 E_0^2 / 4m\Omega^2 + q\Phi, \quad (1)$$

5 where  $E_0$  is the E-field due to the AC voltages,  $\Phi$  is  
 6 the electrostatic potential due to the DC voltages  
 7 and  $R_0$  is the position of an ion averaged over  
 8 several cycles of the AC voltage.

9  
 10 With respect to an electrode, the AC part is always  
 11 repulsive whereas the DC part can be either  
 12 attractive or repulsive.

13  
 14 A DC system alone cannot trap ions since the  
 15 potential has a negative curvature in at least one  
 16 direction. However, the combination of AC and DC  
 17 voltages results in an effective potential that at  
 18 some locations has a positive curvature in all  
 19 directions such that charged particles can be  
 20 trapped.

21  
 22 Equation (1) above can be re-cast as

$$23 \quad V^*(R_0) = qV_{dc}(kE_0^2 + \Phi_r) \quad (2)$$

24  
 25 where a factor of  $q$  has been dropped through  
 26 conversion to electron-volts for the units of  
 27 potential and by considering singly charged ions  
 28 (although the system described here is not subject  
 29 to that limitation).  $k$  has the value  
 30  
 31

$$k = q\gamma^2 / 4m\Omega^2$$

(3)

where  $\gamma$  is a scaling parameter for the AC voltages applied to the system of electrodes, compared to the DC voltage applied, defined explicitly by  $\gamma = V_{ac}/(V_{dc}l)$ , where  $V_{ac}$  and  $V_{dc}$  are the actual voltages applied to the electrodes and  $l$  gives the length-scale associated with the whole design.

The variable  $k$  thus serves as a parameter which can illustrate the scaling of a potential. For a specific trapped particle,  $\gamma$  or  $\Omega$  can be varied. The variables  $q$  and  $m$  are specific to the particle that is trapped.

Thus, in contrast to known particle trapping or guiding techniques, the present invention provides for the trapping or guiding of particles where the trapping electrodes do not have to surround the particle. The electrodes can be arranged in any suitable formation. One option would be for them to lie in a plane. Other options are possible; in particular, the electrodes may be in an array which is substantially planar, but in which some are at relatively raised or lowered positions. The electrodes may also be arranged, for example, in a hemispherical, ellipsoidal or paraboloid configuration.

In a first embodiment, a spot trap is provided. A single electrode is surrounded by a large earth



1 plane. The system is readily scalable through  
2 appropriate scaling of the value of  $k$ .

3  
4 Provided the AC voltage is applied at a frequency  
5 sufficiently low to ensure light can travel across  
6 the system in a time much less than one period, the  
7 potential due to the AC voltage is simply that due  
8 to the DC voltage but modulated in time.

9  
10 Fig. 1 is a plot of the potential contours for a  
11 specific trapping configuration of a circular  
12 electrode. In this system, a  $10\mu\text{m}$  radius spot was  
13 chosen and had a DC voltage of  $-1\text{V}$  applied to it  
14 with respect to the earth plane. The value of the  
15 scaling parameter  $k$  was chosen to be 100.

16  
17 The horizontal ordinate is the perpendicular  
18 distance from the electrode plane and the vertical  
19 ordinate the radial distance from the symmetry axis,  
20 both in  $\mu\text{m}$ . The minimum of the effective potential  
21 (located at approximately  $r=0\mu\text{m}, z=11\mu\text{m}$ ) has a value  
22 of  $-0.186\text{V}$  with respect to the surrounding earth  
23 plane. Contours are shown for  $-0.18$  to  $-0.11\text{V}$  in  
24  $0.01\text{V}$  intervals.

25  
26 Because the system concerned has cylindrical  
27 symmetry about an axis passing through the centre of  
28 the circular electrode and perpendicular to the  
29 plane it is sufficient to demonstrate the resultant  
30 effective potential has the form required to trap  
31 particles in one plane passing through the symmetry  
32 axis to demonstrate the system is an ion trap. It

15

1 can therefore be seen that this is a trapping  
2 configuration.

3  
4 Numerical tests have shown that the system traps  
5 ions for a range of values of  $k$  greater than about  
6 80.

7  
8 The distance of the trap centre from the surface and  
9 the curvature at the bottom of the trap can be  
10 changed by changing the value of  $k$ . In particular,  
11 as the value of  $k$  is increased, particles of a given  
12 mass will be trapped at a point more distant from  
13 the plane of the electrode. As  $k$  is dependent on a  
14 particle's mass, it follows that, for a given value  
15 of  $k$ , particles of heavier mass will lie closer to  
16 the plane of the electrode. Furthermore, as  $k$   
17 increases, the curvature of the bottom of the  
18 potential well changes, resulting in a larger sized  
19 and differently shaped trapping region. Note that  
20 this change in the trapping region is distinct from  
21 the change in trapping region brought about by  
22 funnelling techniques disclosed below, where the  
23 shape of the trapping region remains constant.

24  
25 The ion will remain trapped in the trapping region  
26 provided the adiabaticity parameter is small enough.

27  
28 It is given by

$$\eta = \frac{2q|VE_0|}{m\Omega^2}$$

(4)

29  
30

1 Experiments have shown that this parameter must have  
2 a value of less than 0.3 for stable trapping. Tests  
3 indicate this parameter will have a value of about  
4 0.05 near the minimum of the effective potential so  
5 the trapping is expected to be stable. Further  
6 numerical tests can be made to verify this assertion  
7 and to determine the volume over which stable  
8 trapping occurs.

9  
10 This principle is not restricted to a simple  
11 circular trapping electrode. For example, a matrix  
12 of electrodes could be fabricated. The voltages  
13 applied to the various electrodes can then be chosen  
14 to manipulate particles in a number of ways, some of  
15 which are illustrated below.

16  
17 For example, in a second embodiment, the voltages  
18 applied to the various electrodes in an array could  
19 be chosen for example so that all of those lying  
20 inside a given region are biased with an appropriate  
21 DC voltage and an AC voltage with the remaining  
22 electrodes being biased to zero volts. Gradually  
23 changing the location of the region inside which the  
24 biased electrodes reside (i.e. changing electrodes  
25 successively from being biased to being at earth and  
26 the other way in a systematic fashion) corresponds  
27 to moving the trap location across the surface,  
28 effectively creating a particle conveyor belt.  
29 In a third embodiment, the electrodes can act as a  
30 funnel, the voltages being varied so as to bring  
31 trapped particles from a wide area to be  
32 concentrated in a central region.

1 An example of an electrode configuration that can  
2 act as a funnel is shown in Fig. 2. A series of  
3 concentric electrodes 10 is provided, which  
4 initially all have the same AC and DC voltages  
5 applied. They are surrounded by a large earth plane  
6 12. Thus, in an initial state, the system looks  
7 like a spot-trap, with a diameter equal to  $D_1$ , and  $k$   
8 set to a particular value. After some time in this  
9 configuration, the outer electrode would be set to  
10 0V (making it seem like part of the earth plane),  
11 whilst the waveform applied to the others would be  
12 changed to keep  $k$  at the same predetermined value  
13 (note  $I$  has changed because the diameter of the spot  
14 is equal  $D_2$ ). There is then a first intermediate  
15 state, where the effective potential now has the  
16 same form, but is slightly shrunk in comparison to  
17 the potential in the initial state. Thereafter,  
18 successive electrodes are grounded from the outside  
19 in, always keeping  $k$  constant, until a final state  
20 is reached where the particle is trapped by the  
21 central electrode.

22  
23 An alternative way of funnelling a particle may be  
24 to provide the same electrode structure, but  
25 initially only have the outer few rings with  
26 voltages applied, with those inside being earthed.  
27 Then, moving successively from the outside, each  
28 electrode is set to zero while one more inner has  
29 voltages applied. Thus, the particles are again  
30 focussed in a central region.  
31

1 The innermost electrode can be provided with an  
2 aperture, which acts as an extraction hole. As seen  
3 above, for smaller values of  $k$ , the particles are  
4 trapped closer to the surface of the electrodes. As  
5  $k$  is reduced further, the potential ceases to act as  
6 a trapping potential. At a certain value of  $k$ ,  
7 (found to be 77.7 for the specific spot trap  
8 mentioned above), the trap "breaks" and a trapped  
9 particle can escape. The potential contours at this  
10 point are illustrated in Fig. 3. A biased  
11 extraction electrode can optionally be provided on  
12 the other side of the aperture.

---

13  
14 When the system is used with a buffer gas, the two  
15 sides of the extraction region can be differentially  
16 pumped so that the buffer gas going through the  
17 aperture undergoes a supersonic expansion so that  
18 the beam of particles passing through the aperture  
19 is cooled.

20  
21 In a fourth embodiment, the abovementioned spot trap  
22 and conveyor belt configurations can be combined to  
23 provide manipulation of particles, where particles  
24 of differing mass or charge can be separated and  
25 treated differently.

26  
27 The scaling parameter,  $k$ , is inversely proportional  
28 to the mass of the trapped particles, so that more  
29 massive particles are trapped closer to the surface  
30 of an electrode. Fig. 4 shows a configuration where  
31 a series of conveyor electrodes 14 is provided,  
32 forming a conveyor 16, to which the voltages applied

19

1 allows the conveyor 16 to transport particles from  
2 one trapping region to another. A spot trap  
3 electrode structure 18 is situated in the middle of  
4 the conveyor 16.

5  
6 The relative length scales of the conveyor  
7 electrodes 14 and the spot trap electrodes 18 are  
8 such that the conveyor electrodes 14 are much larger  
9 than the spot trap electrodes 18. When a relatively  
10 light particle is trapped by the spot trap 18, it is  
11 trapped at such a height that, due to the local  
12 nature of the e-field and potential, it is more  
13 influenced by the potential of the conveyor 16 than  
14 the spot trap 18.

15  
16 Hence, one can envisage a system where (possibly  
17 after some interaction) particles arrange themselves  
18 at different distances from the surface depending on  
19 their masses. The less massive particles would then  
20 rise up and be swept away by a conveyor belt, with  
21 the heavier particles remaining in the trap region.

22  
23 After such a process, the remaining heavier  
24 particles could be passed through an extraction  
25 hole, using the methods described above.

26  
27 Alternatively, one might be interested in a process  
28 where the particle mass increases. In this case the  
29 trap could initially be programmed to hold both the  
30 mass before and after an interaction. It then could  
31 be periodically programmed to have a lower value of  
32  $k$  so the lighter (unchanged) particles rise up to be

1 transported to a holding zone. The trap could then  
2 become part of a conveyor belt, perpendicular to the  
3 direction the lighter particles were moved. The  
4 heavier (changed) particles would then be  
5 transported away for further processing after which  
6 the lighter particles could be returned (possibly  
7 with others added) to the interaction region.

8  
9 In a fifth embodiment, where particles are trapped  
10 at a certain height, the value of the scaling  
11 parameter  $k$  can be decreased such that the particles  
12 are lowered towards the electrode surface to  
13 interact with other particles deposited there. The  
14 value of  $k$  can then be increased again so that the  
15 product particles, and any unchanged particles can  
16 be raised up.

17  
18 In all of the above embodiments, printed circuit  
19 board technology can be used to construct the  
20 electrode arrays. The proximity of adjacent  
21 electrodes is limited by cross talk effect, but the  
22 nature of the interactions should be such that  
23 useful devices can be constructed for the  
24 transportation of various particles, such as, for  
25 example, ions or electrons.

26  
27 Indeed, there are many technologies for forming such  
28 arrays, such as focussed ion beam or lithographic  
29 techniques. The choice of construction method will  
30 depend on the length scale and application of the  
31 particular array to be constructed.

32

1 The above concepts have a wide range of potential  
2 applications. In particular, the techniques above  
3 may be used to enable miniaturisation and  
4 parallelisation of current techniques for frequency  
5 standards, quantum computation, quantum encryption  
6 and material analysis.

7  
8 In addition, the techniques are directly applicable  
9 to the manufacture of devices for manipulating ions,  
10 for use in high end biomolecular experiments.

11  
12 It will be appreciated that the electrodes of an  
13 apparatus, which are connected to an appropriate  
14 power supply, will normally be contained within a  
15 sealable chamber, and a gas pump is provided to  
16 introduce and extract gas in order to vary the  
17 pressure and control the quality of vacuum provided  
18 in the chamber.

19  
20 Fig. 5 shows an apparatus that uses the techniques  
21 of the present invention, which is particularly  
22 intended to be used with biomolecular ions.

23  
24 Ions 20 are introduced into a chamber 24. Optional  
25 gate electrodes 22 are used to control the  
26 introduction of the ions 20. The ions 20 are used  
27 to seed an array of trap electrodes 26.

28  
29 A pump and gas inlet valve (not shown) control the  
30 introduction and extraction of a background buffer  
31 gas, to control the vacuum provided by the chamber  
32 24.



1 The voltages applied to the array 26 can be varied  
2 to manipulate ions 20, as described above. At any  
3 time, the trapping voltages can be switched off and  
4 an extraction voltage can be applied to an  
5 extraction plate 28 to accelerate the ions 20  
6 through a flight tube 30 towards a position-  
7 sensitive detector 32. Although the ions 20 may  
8 undergo several collisions in the flight tube 30  
9 these collisions will be brief and with the much  
10 lighter buffer gas partners. Accordingly these  
11 collisions should not destroy the positional or  
12 time-of-flight information.  
13  
14 Time-of flight will be used to distinguish genuinely  
15 trapped or guided ions 20 from background ions so  
16 the time-gated image on the position-sensitive  
17 detector 32 corresponds to a snap-shot of the ion 20  
18 locations just prior to the application of the  
19 extraction voltage.  
20  
21 It will be appreciated that trapped ions have a  
22 thermal energy distribution that means they will  
23 have a finite chance of escaping, much as a water  
24 molecule has a chance of evaporating from a liquid  
25 below the boiling point. When such a trapped  
26 particle escapes, it passes through the aperture.  
27 However, as the voltages are varied, this shall  
28 occur slightly before the normally expected  
29 transmission time of that particular particle. The  
30 times when a particle may escape outside of these  
31 transmission times will depend on the values and  
32 rate of changes of the amplitude, waveform, and

1 frequency of the voltages applied. Thus, the mass  
2 of the particle can be determined by correlating the  
3 time of passage through the aperture with the state  
4 of the trap at that time.

5  
6 Various buffer gas collision regimes can be  
7 explored, particularly the high collision frequency  
8 limit (useful for material processing and working  
9 with Biomolecules) and the collisionless limit  
10 (useful for quantum computation and encryption). In  
11 the high frequency limit the ions will rapidly  
12 become thermalised through collisions with  
13 background gas and one another. This background can  
14 be a rare gas buffer so no unwanted chemical  
15 reactions occur, or it could be, for example, water  
16 to investigate hydration of biomolecules. A rare  
17 gas buffer can easily be cooled to liquid N<sub>2</sub>  
18 temperature when the characteristic energy  
19 associated with each degree of freedom will be about  
20 3meV so the trapped ions will lie inside the  
21 trapping region, which is seen as the innermost  
22 contour of Fig. 1.

23  
24 The details of the dynamics in the collisionless  
25 limit are harder to calculate although this can be  
26 done using certain computer simulation techniques.

27  
28 For a given voltage configuration the motion of a  
29 single ion can be approximated by a superposition of  
30 harmonic motions, which may be coupled.  
31

1 Another device that can be constructed using the  
2 principles of the invention is a single  
3 reconfigurable trap. This can be a few centimetres  
4 across, with circular electrodes centred about an  
5 extraction region consisting of a small aperture  
6 with the trap system to one side and a biased  
7 extraction electrode to the other side. For such a  
8 trap, the effective potential takes the form shown  
9 in Fig. 1. The effective potential contours are  
10 chosen so that the innermost contour corresponds to  
11 room temperature, compared to the minimum.

12  
13 The trap will be gradually reconfigured so that the  
14 length scale gradually reduces from about 3cm to  
15 50 $\mu$ m, so all of the ions trapped in the potential  
16 are gathered into a successively smaller volume,  
17 similar to a deflating balloon.

18  
19 The trapping nature will then be changed so that the  
20 ions are free to move towards the extraction region,  
21 centred at the origin. The potential will take the  
22 form shown in Fig. 3 (note change in z-axis), when  
23 the trapped ions will escape through the extraction  
24 region. The two sides of the extraction region can  
25 be differentially pumped so the buffer gas going  
26 through the aperture will undergo a supersonic  
27 expansion giving further cooling to the beam of  
28 biomolecular ions.

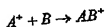
29  
30 The resultant pulsed source of cold biomolecular  
31 ions will be ideal for investigating their reactive

1 scattering behaviour, hence creating a new and  
2 topical research field.

3  
4 The principles of the present invention can also be  
5 used to construct a position-sensitive detector,  
6 which is illustrated in Fig. 6.

7  
8 An array of traps 34 forms a planar electrode  
9 structure 36 and is loaded with a specific molecular  
10 ion ( $A^+$ ) chosen to be able to react associatively  
11 with a particular biomolecule or class of  
12 biomolecules (B). The choice of  $A^+$  relates to the  
13 specificity of the detector. A microchannel plate  
14 40 is provided, the front surface of which is biased  
15 highly negatively to attract the positive ions.  
16 Alternatively, any suitable position sensitive  
17 charged particle detector may be used in place of a  
18 microchannel plate.

19  
20 When a molecule B approaches the planar structure 36  
21 it can then react with one of the sensor molecule  
22 ions in the associative reaction:



(5)

23  
24  
25  
26 The trap configuration is arranged so that the  
27 product ion, being more massive falls towards the  
28 electrode surface 36 eventually being swept through  
29 due to a field penetrating through one of an array  
30 of small holes 38. This penetrating field occurs as  
31 a natural consequence of biasing the front surface  
32 of the microchannel plates 40 highly negative. Note

1 that the same effect could be achieved by having the  
2 back face of the electrode array being negatively  
3 charged. The ion is then accelerated from the hole  
4 38 towards a microchannel plate 40, which will be  
5 the front-end of a traditional position sensitive  
6 detector (something akin to an image intensifier).  
7 The resultant detection event provides a record of  
8 the position of the biomolecule prior to the  
9 interaction.

10  
11 It may additionally be possible to cycle the  
12 trapping so that the more massive product ions are  
13 held in the trap and can only reach the penetrating  
14 field periodically. In this case, time-of-flight  
15 information can be used to determine the mass of the  
16 product ion and hence determine the mass of  $A^+$  as  
17 well as the class of molecules to which it belongs.

18  
19 The innate capability of the trapping array to store  
20 different ions at different locations could be  
21 exploited to store different species  $A^+$  at different  
22 locations, making the system able to distinguish a  
23 range of biomolecules (B) simultaneously.

24  
25 A bespoke CAD/simulation package can also be  
26 provided to aid in the design of arrays to trap or  
27 guide charged particles. For a given trap  
28 configuration subject to any sequence of applied  
29 voltages, the motion of trapped ions can in  
30 principle be solved exactly through solution of  
31 Maxwell's equations for the fields and Newton's  
32 equations for the motion of the ions. However, this

1 might be computationally intractable for the scale  
2 of problems envisaged.

3  
4 Because of the length and frequency scales involved,  
5 linear combinations of solutions of Laplace's  
6 equation can be used in place of the full solution  
7 of Maxwell's equations. This problem is  
8 computationally tractable for arbitrary geometries  
9 and, due to the near-symmetries of the trap arrays  
10 proposed, amenable to further speed-ups through  
11 multi-resolution analysis. Using solutions of  
12 Laplace's equation obtained in this manner, the  
13 properties of the trapping or guiding arrays will be  
14 deduced by solving the dynamics of the trapped ions  
15 at various levels of approximation ranging from full  
16 explicit solution of the motion of trapped ions  
17 coupled to a Monte-Carlo simulation for collisions  
18 with the buffer gas (computationally expensive) to  
19 simply calculating the effective trapping potential  
20 averaged over a particular 'trapping sequence' of  
21 applied voltages and then using statistical  
22 distributions and friction models for the ions  
23 subject to this effective potential (computationally  
24 cheap).

25  
26 Such simulations will first be used to assess the  
27 range of validity of computationally cheap  
28 strategies. Once this is established, the effective  
29 potential and adiabaticity parameter for various  
30 trap/guide configurations and 'trapping sequences'  
31 will be used to predict their behaviour.  
32

1 Control of the program will be achieved through a  
2 visual interface, leading to a bespoke  
3 CAD/simulation program for ion trap/guide arrays,  
4 which can be made available to researchers in the  
5 field, and can act over an array of PC's acting as a  
6 parallel computer. Both the solution of Laplace's  
7 equation and the calculation of trajectories are  
8 amenable to parallel computation.

9  
10 Various modifications can be made without departing  
11 from the scope of the present invention. In  
12 particular, the charged particles may comprise ions,  
13 electrons, or any other suitable charged particles.

14  
15 The fabrication of the electrode arrays may be by  
16 any suitable means, of which printed circuit board  
17 technology, lithographic methods, and focussed ion  
18 beam methods are examples only.

19  
20 The shape of electrodes in each embodiment may take  
21 any suitable shape, and the examples given should  
22 not be taken as limiting these to any particular  
23 shape. For example, a funnel configuration could be  
24 implemented by means of a series of concentric  
25 circular electrodes. These electrodes could be  
26 ellipsoidal, square, or any other suitable shape.

27  
28 The voltages applied to the electrodes may take any  
29 suitable form, and can be modulated before being  
30 sent to the electrodes. For example, the voltages  
31 could be square waves to enable digital logic  
32 techniques to be used when processing the

1 information. Furthermore, the voltages applied to  
2 the electrodes can be of appropriate polarity to  
3 attract or repel specific particles. For example,  
4 in the apparatus for carrying out the method of the  
5 sixth embodiment, the microchannel plate is biased  
6 negatively. However, it could be charged positively  
7 to attract negative particles.

8  
9 It will also be acknowledged that in configurations  
10 such as the conveyor belt, their operation is  
11 described in terms of actually transporting  
12 particles; however the voltage sequences can be  
13 applied even when no particles are present, so that  
14 the conveyor configuration may be always active, to  
15 transport particles as and when they are present.

16  
17 It will also be appreciated that specific  
18 applications of the principles of the invention may  
19 be applied in combination.



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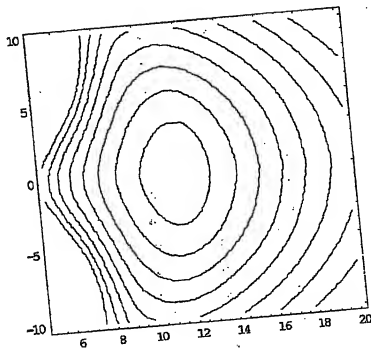


Figure 1

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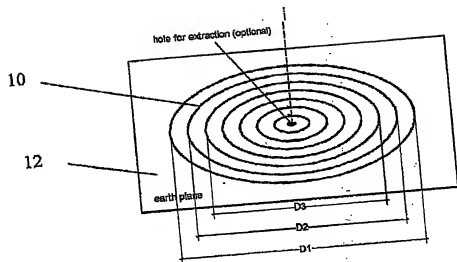


Figure 2

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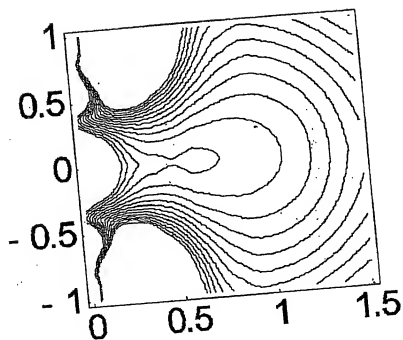


Figure 3

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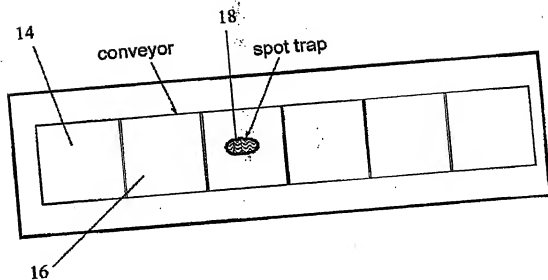


Figure 4

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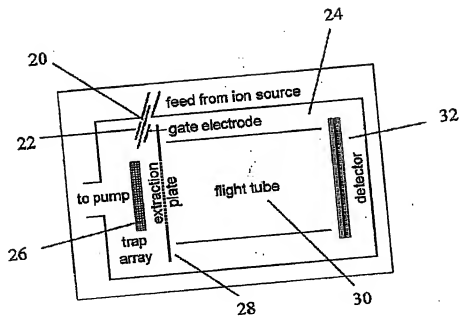


Figure 5

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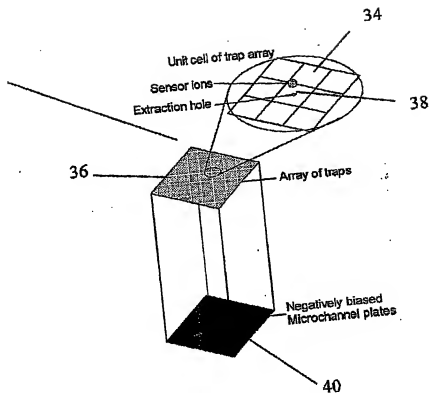


Figure 6



PCT Application

**GB0303683**



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